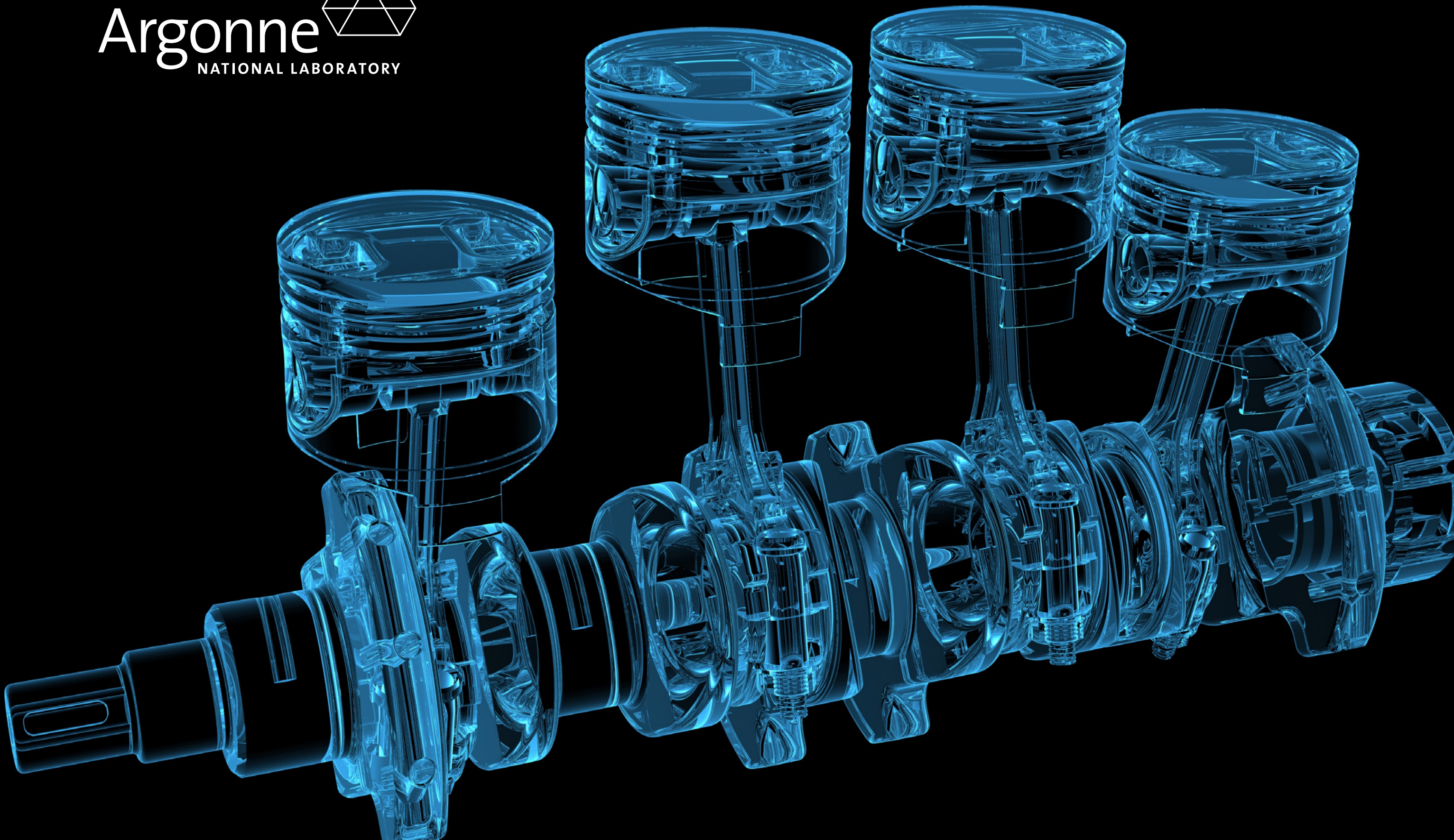
Argonne NATIONAL LABORATORY



Ushering in a New Era of

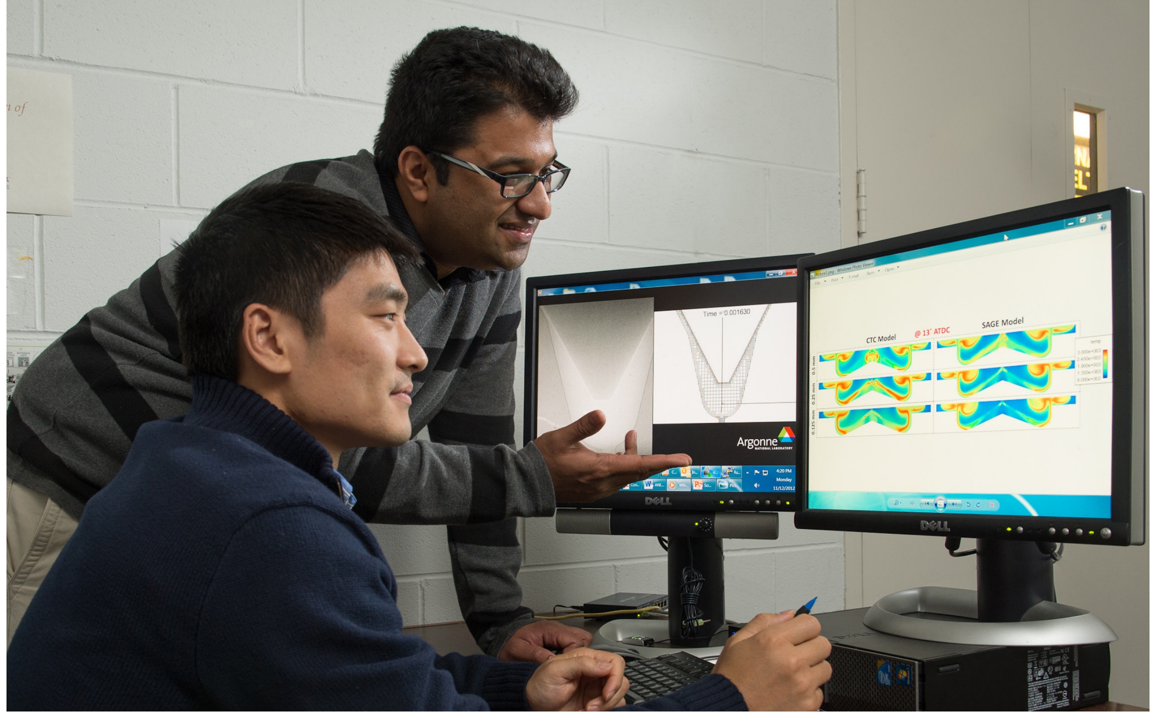
Intelligent Engine Design

Ushering in a New Era of Intelligent Engine Design

"The use of predictive simulation tools for enhancing combustion engine performance will shrink engine development timescales, accelerate time to market, and reduce development costs, while ensuring the timely achievement of energy security and emissions targets and enhancing U.S. industrial competitiveness."

– From the U.S. Department of Energy's Predictive Simulation for Internal Combustion Engines (PreSICE) workshop report (March 3, 2011). The workshop was attended by more than 60 U.S. leaders in the engine combustion field from industry, academia, and national laboratories.

Improving the fuel efficiency of internal combustion engines is **critical** to **reducing U.S. dependence on petroleum** and **decreasing greenhouse gas emissions**. While gasoline and diesel engines continue to see incremental improvements in fuel economy, understanding and controlling fuel sprays and stochastic in-cylinder processes are the **most significant barriers** to **enhancing engine efficiency**. However, these hidden-from-view processes can only be optimized with the help of **cutting-edge predictive modeling** and **simulation tools**.

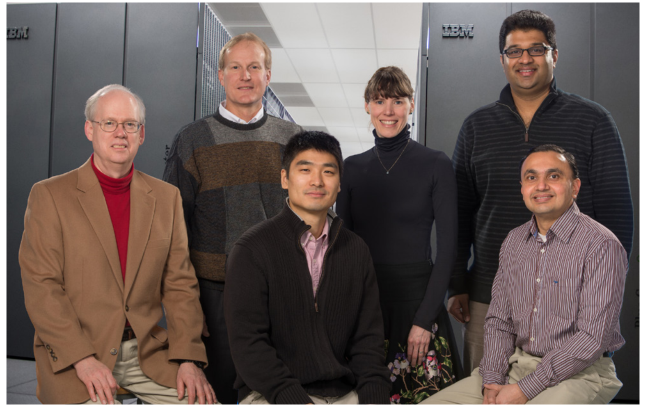


Argonne researchers Qingluan Xue (foreground) and Sibendu Som discuss simulation results.

The traditional "build and test" prototype approach to automotive engine design and development is time consuming and expensive. The U.S. Department of Energy's Predictive Simulation for Internal Combustion Engines (PreSICE) workshop concluded that industry practices must be dramatically accelerated to help improve vehicle fuel economy, thus reducing our nation's petroleum dependency and carbon emissions.

Researchers at Argonne National Laboratory are opening the door to a new era of intelligent engine design with their work to develop more robust predictive engine simulations, providing industry with an improved and accelerated path to more fuel-efficient and clean automotive engines.

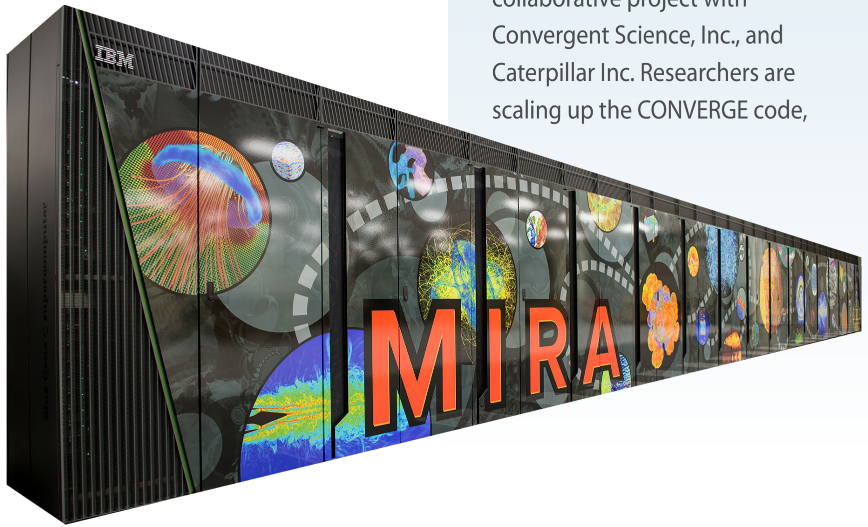
With expertise in automotive engines and combustion chemistry, and state-of-the-art transportation and high-performance computing (HPC) facilities, Argonne's well-rounded program is enabling researchers to rapidly advance computational tools, including improved fuel spray and combustion models, for high-performance, massively parallel computing systems.



From left, Argonne researchers Raymond Bair, Doug Longman, Qingluan Xue, Marta Garcia, Shashi Aithal (seated) and Sibendu Som are part of a multidisciplinary team working to advance diesel and spark engine modeling and simulation tools into the high-performance computing realm.

Using HPC capabilities at the Argonne Leadership Computing Facility, Argonne researchers are elevating engine modeling and simulation capabilities to new heights. The laboratory's multidisciplinary research team has already run the **largest diesel engine simulations ever performed**. And soon, they will surpass this feat using Argonne's Mira supercomputer, one of the fastest computers in the world. This groundbreaking work is part of a collaborative project with Convergent Science, Inc., and Caterpillar Inc. Researchers are scaling up the CONVERGE code, a software program widely used by industry, to **run on high-performance computers without any technical glitches**.

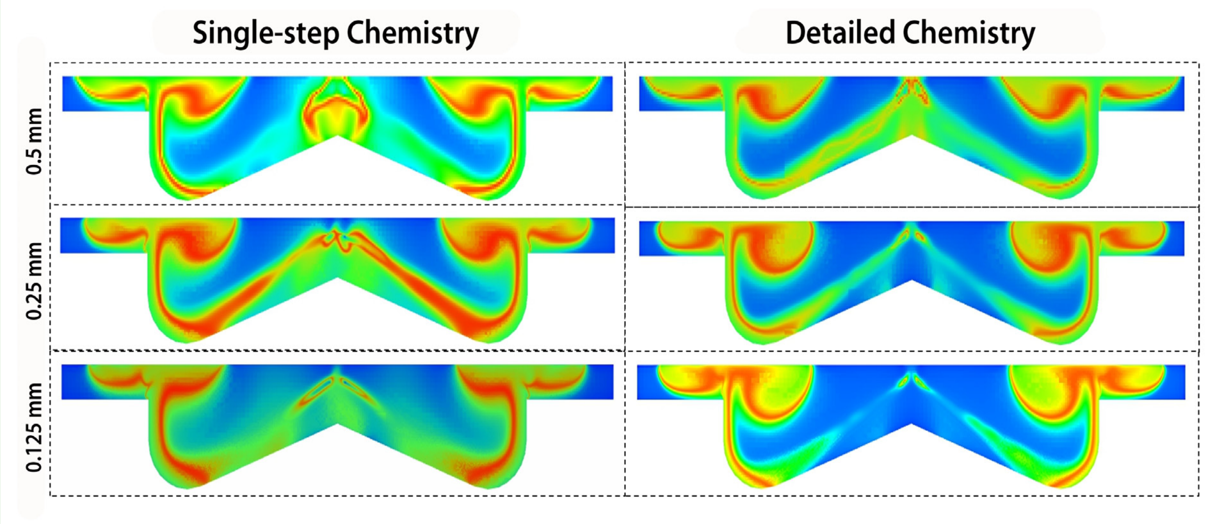
The current state-of-the-art for most manufacturers involves running engine simulations with up to 50 processors. The Argonne team has modified CONVERGE to run effectively on more than 1,000 processors. This huge leap forward was made possible by the development and implementation of an improved load-balancing algorithm called METIS (original algorithm developed at University of Minnesota). The massive engine simulations have also successfully demonstrated grid convergence on several engine combustion parameters. Work continues to expand the code for Mira.



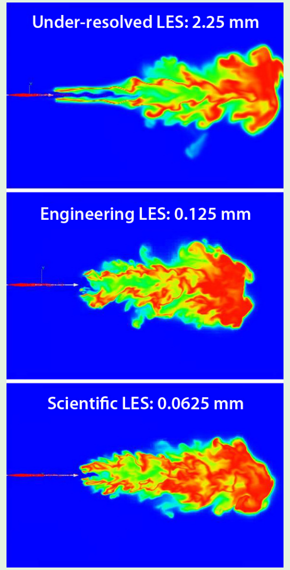
Mira, Argonne's new supercomputer, is a 10-petaflop IBM Blue Gene/Q system capable of 10 quadrillion calculations per second.

The combustion process depends on a complex web of chemical reactions. Argonne chemists are working to understand and characterize these reactions for a variety of fuels over a wide range of temperatures and pressures. Combining theoretical and experimental efforts, their research is **providing insight into key chemical reactions and coupled kinetics processes**. The resulting chemical models are ultimately implemented into computer simulations to predict and optimize the performance of internal combustion engines.

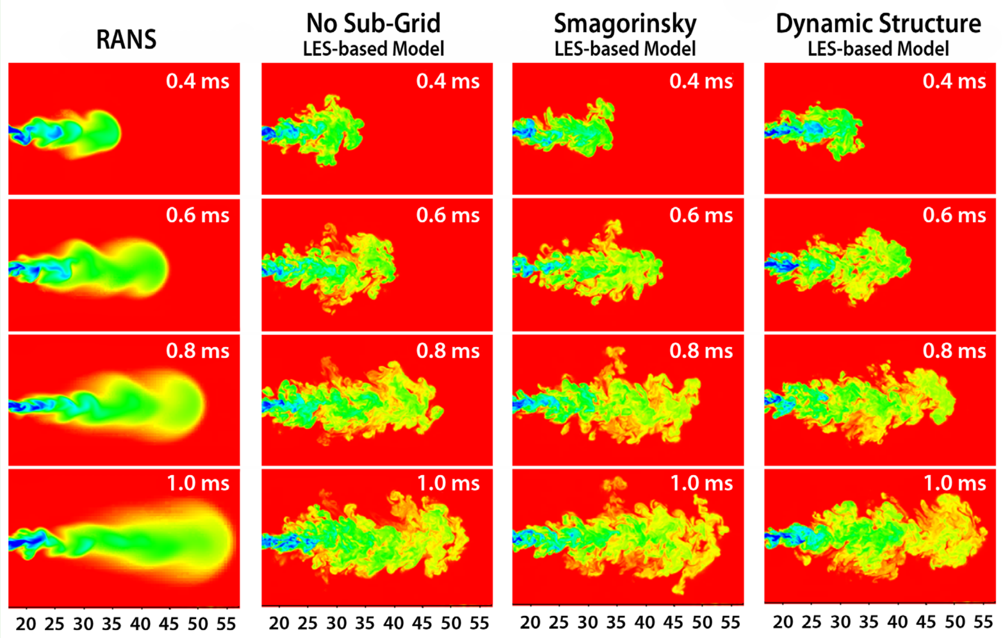
In collaboration with University of Connecticut and Lawrence Livermore National Laboratory, Argonne researchers have developed high-fidelity reduced mechanisms for diesel and biodiesel fuel surrogates. These improved chemical kinetic models are now benchmarked and **available to the industry for in-house engine simulations**.



The temperatures inside the combustion chamber predicted by single-step and detailed chemistry based combustion models are significantly different.



The temperature distribution inside the combustion chamber of a diesel engine obtained using high-fidelity simulations and a robust, large-eddy simulation model.

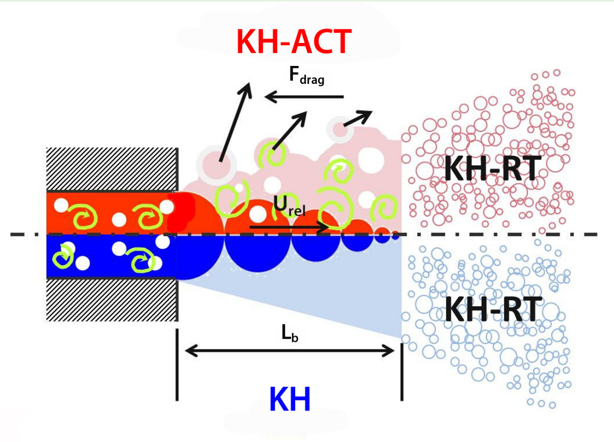


The effect of different turbulence models on fuel and temperature distribution inside the combustion chamber can be seen here. The degree of complexity of the turbulence model increases from left to right. The Dynamic Structure model captures more flow structures compared to the other models.

Optimizing combustion also requires a fundamental understanding of the turbulent mixing of fuel and air that takes place at the molecular level. Combining HPC resources with the large-eddy simulation (LES) techniques, Argonne researchers in collaboration with Convergent Science, Inc., have demonstrated a **new approach to turbulence modeling that sheds more light on the flow processes taking place in engines**. LES, a widely used technique for modeling turbulent flows, is a valuable tool for capturing fuel spray dynamics and the variations that occur in the combustion process from cycle to cycle. Argonne's work has shown that LES **improves qualitative and quantitative predictions** of factors such as equivalence ratio distributions, ignition delay and soot distribution.

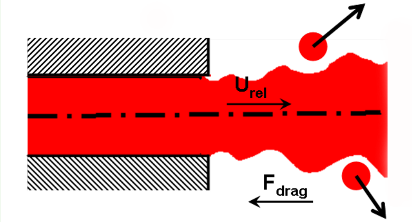
Primary fuel atomization is induced by aerodynamics in the near-nozzle region as well as cavitation and turbulence from the injector nozzle. The traditional breakup models used in diesel engine simulations generally consider aerodynamically induced breakup using the Kelvin-Helmholtz (KH) instability model, but it does not account for in-nozzle flow effects.

To improve this approach, Argonne researchers **developed the Kelvin-Helmholtz-Aerodynamics Cavitation Turbulence (KH-ACT) model** to cover the impact of cavitation and turbulence effects along with aerodynamically induced breakup. In collaboration with the University of Illinois at Chicago and Convergent Science, Inc., the KH-ACT model was incorporated into the CONVERGE code, presenting **a novel tool for industry** to capture the influence of in-nozzle flow and fuel properties on spray, combustion and emission processes.

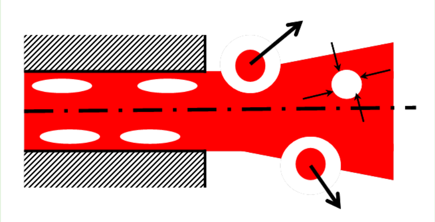


Implementation of the KH-ACT primary breakup model.

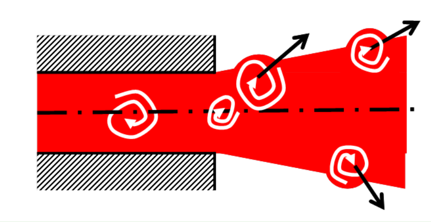
Near-nozzle Breakup Mechanisms



Aerodynamically induced

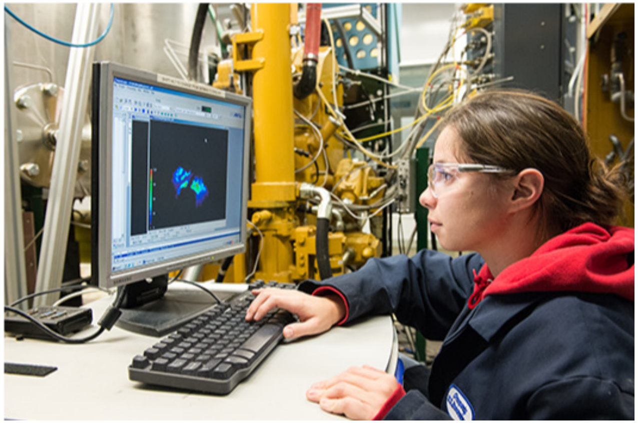


Cavitation-induced



Turbulence-induced

Validation



Argonne engineer Anita Ramirez performs dynamometer tests on a single-cylinder Caterpillar engine to validate data for the modeling and simulation efforts.

Argonne engineer Doug Longman uses a volt meter to check the engine's electronic system.

The modeling team works closely with researchers at Argonne's Advanced Photon Source (APS) and the laboratory's Engine Research Facility to **validate simulation data against precise measurements**, under well-controlled operating conditions.

At the APS, scientists are using the facility's powerful X-ray beams to peer deep inside the detailed structure of sprays from diesel and gasoline fuel injectors. Engineers at the Engine Research Facility run engine dynamometer tests to study in-cylinder combustion and emissions under realistic conditions. Results from these efforts, along with findings from other national laboratories, **provide the benchmark data necessary for model validation**.

For more information, contact

Sibendu Som
ssom@anl.gov

Doug Longman
dlongman@anl.gov

U.S. DEPARTMENT OF ENERGY

Argonne National Laboratory is a U.S. Department of Energy laboratory managed by U Chicago Argonne, LLC.